Physics of the Solid State 2003 vol.45 N5, pages 854-858

# First-principles calculations of the hyperfine fields on ligands in fluorides

Anikeenok O.
*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

## Abstract

In solid-state physics, a crystal lattice is frequently approximated by an array of interacting ions. In this case, the wave functions of individual ions are assumed to be a fairly good zeroth approximation in calculating the matrix elements of the interaction Hamiltonian of electrons and nuclei of the lattice from first principles. Use of the second-quantization method is proposed for such calculations in the basis of these functions. As an example, the electron transition amplitude from a ligand to the central ion is estimated. The results agree well with the experimental data. © 2003 MAIK "Nauka/Interperiodica".

http://dx.doi.org/10.1134/1.1575322